Valeranone

Inchi: InChI=1S/C15H26O/c1-11(2)12-7-9-14(3)8-5-6-13(16)15(14,4)10-12/h11-12H,5-10H2,1-4
InchiKey: HDVXJTYHXDVWQO-SNPRPXQTSA-N
Formula: C15H26O
SMILES: CC(C)C1CCC2(C)CCCC(=O)C2(C)C1
Mol. weight [g/mol]: 222.37
CAS: 55528-90-0

Physical Properties

Property code	Value	Unit	Source
gf	4.80	kJ/mol	Joback Method
hf	-364.81	kJ/mol	Joback Method
hfus	6.94	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.208		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1668.00		NIST Webbook

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rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1671.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1667.60		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1662.00		NIST Webbook
ripol	2155.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2145.00		NIST Webbook
ripol	2145.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2128.00		NIST Webbook
ripol	2144.00		NIST Webbook
tb	636.35	K	Joback Method
tc	876.05	K	Joback Method
tf	377.39	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.33	J/mol×K	636.35	Joback Method
cpg	606.66	J/mol×K	676.30	Joback Method
cpg	629.73	J/mol×K	716.25	Joback Method
cpg	651.81	J/mol×K	756.20	Joback Method
cpg	673.17	J/mol×K	796.15	Joback Method
cpg	694.07	J/mol×K	836.10	Joback Method
cpg	714.79	J/mol×K	876.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55528900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume